Isopropanol

67-63-0 | DTXSID7020762

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 6.10e-01

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 8.46e-01

Nearest Neighbors from the Training Set

Image not found

tert-Butyl alcohol
Measured: 0.7
Predicted: 6.52e-01

Image not found

Dimethyl sulfoxide
Measured: 0.6
Predicted: 6.10e-01

Image not found

Diethyl ether
Measured: 0.73
Predicted: 6.74e-01

Image not found

3-Pyridinamine
Measured: 0.32
Predicted: 4.83e-01

Image not found

4-Aminopyridine
Measured: 0.66
Predicted: 4.83e-01